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A Consistent Prescription for Combining Perturbative Calculations and Parton Showers in Case of Associated $\mathrm{Z^0 b\bar{b}}$ Hadroproduction

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Abstract: This paper presents the method of combining parton shower formalism with perturbative calculations (matrix elements) in form of a Monte-Carlo algorithm for the process $gg \to Z^0/\gamma^* b\bar{b}$, consistently including the heavy quark masses and overlap removal.

Keywords: QCD, NLO Computations, Parton Model, Hadronic Colliders.

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Contents

1. Introduction

The $gg \to Z^0/\gamma^* b\bar{b} \to f\bar{f}b\bar{b}$ process is of high experimental interest in view of the forthcoming LHC experiments, since it e.g. represents an irreducible background to the 'gold-plated' Higgs channel $H \to ZZ^{(*)} \to 4$ leptons (see e.g. [1]). Historically, the process has been fully calculated at tree level by Kleiss and Stirling [2] and for the first time successfully implemented inside the AcerMC [3] Monte-Carlo generator. In the present time there is a plethora of other Monte-Carlo generators implementing this process in various advanced fashions (see e.g. [4]), however a few issues still need to be resolved in a consistent fashion:

- At tree level the $gg \to Z^0/\gamma^* b\bar{b} \to f\bar{f}b\bar{b}$ process is actually NNLO in α_s with respect to the order α_s^0 'pure' Drell-Yan process $b\bar{b} \to Z^0/\gamma^* \to f\bar{f}$. The same final state can thus be achieved by using the Sudakov parton showering procedure, which by definition re-sums the large logs of the order $\alpha_s \ln M_Z^2/m_b^2$ which burden the higher order corrections as the $gg \to Z^0/\gamma^* b\bar{b}$ and might thus be better at least in the 'intermediate' kinematic regions (see e.g. [5] where the $gg \to Z^0/\gamma^* b\bar{b} \to f\bar{f}b\bar{b}$ process was actually removed with this argument). While the argument by all means stands it would nevertheless be preferable to have the processes consistently combined in orders α_s^n, $n = 0, 1, 2$, achieving the undisputed validity over the whole phase-space.

- The b-quarks are reasonably massive; still it is customary to treat all partons incoming to the hard process as massless, which is strictly speaking consistent only if

also the final state b-quarks are also treated as massless. In ‘full’ Monte-Carlo procedures, where the produced b-quarks are further hadronized into jets, the mass of the b-quark needs to be present and is thus added in and *ad-hoc* fashion. Furthermore, neglecting the heavy quark masses of the incoming quarks has been shown to have an observable impact and can in fact be consistently added into the Factorization Theorem [7, 8, 9].

The existing prescriptions deal either with massive particles [7, 8, 9] on the level of integrated cross-sections or with explicit Monte-Carlo algorithms involving light ($\sim$ massless) particles (e.g. [4, 5, 10, 11, 12, 13]) while a first attempt at the combination of the two was attempted in the paper [14], where an algorithm combining the two features was developed but implemented only in terms of order α_s^1 correction while for the $gg \to Z^0/\gamma^* b\bar{b}$ process the order α_s^2 combination procedure is needed. The aim of this paper is to show that the procedure developed in [14] is in fact iterative and can thus provide a consistent procedure applicable (at least) at tree-level which can be and is implemented in terms of a full $gg \to Z^0/\gamma^* b\bar{b}$ Monte-Carlo procedure.

2. Combining the Perturbative QCD and Sudakov Showering in Massive Hadroproduction

2.1 Theoretical Basis

Let us start by repeating the considerations of the Factorization Theorem [6, 15, 16, 17, 18], which states that the hadronic cross cross section $\sigma_{\mathrm{AB}\to\mathrm{X}}$ is related to the perturbatively calculated (e.g. by using Feynman diagram technique) parton level-cross section $\sigma_{\mathrm{ab}\to\mathrm{X}}$ by:

$$\sigma_{\mathrm{AB}\to\mathrm{X}} = \sum_{a,b} f_{a/A} \otimes \hat{\sigma}_{ab\to X} \otimes f_{b/B}, \tag{2.1}$$

with $f_{i/I} = f_{i/I}(x, \mu_F)$ denoting the parton density functions (PDF), giving a probability that a fully evolved parton i is produced by the parent hadron I, at the factorization scale μ_F with a certain energy fraction x. The PDFs are convoluted with the *hard* parton-level cross section $\hat{\sigma}_{ab\to X}$ which can in general differ from the perturbative (pQCD) parton level-cross section $\sigma_{\mathrm{ab}\to\mathrm{X}}$.

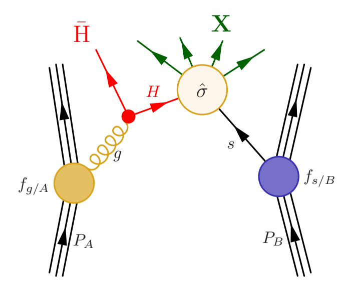

Figure 1: Schematic representation of the example of a gluon splitting $g \to H\bar{H}$ combined with a hard subprocess $\hat{\sigma}$.

Note that the term *hard cross section* in the above application of the Factorization Theorem demands that the hard cross section expression of Eq. 2.1 is indeed describing the *hard* (’short-distance’, high energy) process only, i.e. all the ’long-distance’ contributions in form of collinear/mass singularities and corresponding large logarithms in form of $\alpha_s \log(\mu_F^2/m^2)$ need have been explicitly subtracted since they are already included (resummed) in the PDFs [6, 7, 8]. The factorization scale μ_F sets the dividing limit between the two kinematic regimes.

Let us illustrate how this applies to the case studied in this paper: In a perturbative calculation of order α_s^n an incoming gluon splits to a heavy quark pair $g \to H\bar{H}$; the other incoming parton we mark as the spectator s (c.f. Figure 1). The Factorization theorem then gives:

$$\sigma^{(n)}_{\mathrm{AB}\to\mathrm{X}\bar{\mathrm{H}}} = f_{g/A} \otimes \hat{\sigma}^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} \otimes f_{s/B}\,. \tag{2.2}$$

Possible summations and permutations of incoming flavors are omitted and only the convolution with the parton density functions remains explicit.

Stipulating that the (hard/soft) scale μ is set by the heavy quark kinematics (e.g. heavy quark propagator; other choices are possible) then :

- If the scale is hard enough, $\mu > \mu_F$, the pQCD calculation need not be modified, i.e.

  $$\hat{\sigma}^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} = \sigma^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} \qquad (\mu > \mu_F) \tag{2.3}$$

  in this kinematic region.

- if the scale is soft, $\mu < \mu_F$, the heavy quark production in gluon splitting is 'long-distance' and thus already included in the PDF $f_{H/I}$. In other words, the incoming gluon cannot be resolved at this scale μ_F and the heavy quark H should be considered as the incoming (fully evolved) parton. One should thus use an alternative calculation $\hat{\sigma}^{(n-1)}_{Hs\to X}$ with an incoming quark H instead:

  $$\sigma^{(n-1)}_{\mathrm{AB}\to\mathrm{X}} = f_{H/A} \otimes \hat{\sigma}^{(n-1)}_{\mathrm{Hs}\to\mathrm{X}} \otimes f_{s/B} \qquad (\mu < \mu_F) \tag{2.4}$$

  and correct the perturbative calculation correspondingly.

The latter case ($\mu < \mu_F$) however needs to be explained a bit further: One should *not* simply set $\hat{\sigma}^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} = 0$ since only the collinear kinematic limit (explicit large logs $\alpha_s \log(\mu_F^2/m^2)$) is resummed in the $f_{H/I}$, whereas such logs are only a part (limit) of the full pQCD calculation $\hat{\sigma}^{(n)}_{gs\to X\bar{H}}$ and it is only these contributions that need to be removed in order to prevent double counting of the inclusive $\hat{\sigma}^{(n-1)}_{Hs\to X}$ contribution in this kinematic region. Instead one should put:

$$\hat{\sigma}^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} = \sigma^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} - \sigma^{(n)}_{\mathrm{subt}}, \tag{2.5}$$

which can then be used in the hadronic cross-section expression:

$$\sigma^{(n)}_{\mathrm{AB}\to\mathrm{X}\bar{\mathrm{H}}} = f_{g/A} \otimes \hat{\sigma}^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} \otimes f_{s/B} = f_{g/A} \otimes \sigma^{(n)}_{\mathrm{gs}\to\mathrm{X}\bar{\mathrm{H}}} \otimes f_{s/B} - f_{g/A} \otimes \sigma^{(n)}_{\mathrm{subt}} \otimes f_{s/B}\,. \tag{2.6}$$

One can immediately deduce one property of the subtraction term from Equation 2.3:

$$\sigma^{(n)}_{\mathrm{subt}} = 0 \qquad (\mu > \mu_F). \tag{2.7}$$

The full (correct) cross section involving the heavy flavour excitation in the initial state (category HE in the paper [9]) thus needs the addition of the $\hat{\sigma}^{(n-1)}_{Hs\to X}$ hard process to

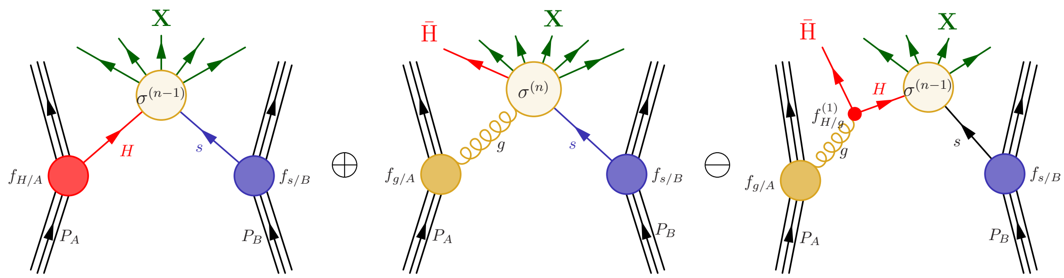

Figure 2: Schematic representation of heavy quark H entering the perturbative calculation at order (n-1) as fully evolved (left) or participating internally via the splitting of the incoming gluon at order (n) (middle) with the appropriate subtraction term (right). The subscript s denotes the other incoming parton (which can also be a heavy quark) and X the inclusive final state.

correctly cover the soft region:

$$\begin{aligned}\sigma_{\mathrm{AB\to X(\bar{H})}} &= f_{g/A} \otimes \sigma^{(n)}_{\mathrm{gs\to X\bar{H}}} \otimes f_{s/B} \\ &- f_{g/A} \otimes \sigma^{(n)}_{\mathrm{subt}} \otimes f_{s/B} \\ &+ f_{H/A} \otimes \hat{\sigma}^{(n-1)}_{\mathrm{Hs\to X}} \otimes f_{s/B}\,, \qquad (\mu < \mu_F)\end{aligned} \tag{2.8}$$

as illustrated also in Figure 2.

At this point it should be emphasised that all the above hadronic cross-sections are *effectively of the same order* if one considers that the heavy quark density $f_{H/I}$ is of the effective order α_s higher with respect to the dominant (gluon or valence quark) parton distribution functions (see e.g. [9] for details). Also note that the final state heavy quark $\bar{H}$ need not be resolved in the final state since both final states $X\bar{H}$ and X from the two hard contributions participate in the full expression of Equation 2.8 and the $\bar{H}$ can in the second case appear only in the soft (parton showering) processes.

An excellent basis for deriving the desired rules and expressions is the paper of Olness, Scalise and Tung [9], which presents a comprehensive review of the formalism needed for obtaining the fully infra-red safe hard cross-sections with the emphasis on isolating and subtracting the divergences related to the heavy quark terms. The derivation of [9] (or equivalently [18] and our previous paper [14]) gives the expression for the subtraction term of the order (n) as (please consult the Appendix A for details):

$$\sigma^{(n)}_{\mathrm{subt}} = f^{(1)}_{H/g} \otimes \hat{\sigma}^{(n-1)}_{\mathrm{Hs\to X}}\,, \qquad (\mu < \mu_F) \tag{2.9}$$

where the first-order in α_s term $f^{(1)}_{H/g}$ is the perturbatively calculated parton distribution function $f^{(1)}_{i/j}$ of a parton *inside another parton* which is explicitly given as (c.f. [9, 14]) :

$$f^{(1)}_{i/j}(\xi,\mu) = \frac{\alpha_s(\mu)}{2\pi} P_{j\to i}(\xi) \ln\left(\frac{\mu^2}{m_H^2}\right) \tag{2.10}$$

with $P_{j\to i}$ being the well-known splitting kernels and also contains the explicit massive divergence logarithm.

This is not necessarily the final step one needs to make to be able to evaluate the hadronic cross sections, since e.g. the spectator s can also be a gluon splitting to heavy quarks (as is indeed the case in the studied $gg \to Z^0/\gamma^* b\bar{b}$ process) and thus the whole procedure and calculation of the subtraction terms needs to be recursively (iteratively) repeated for both n^{th} and $(\mathrm{n}\text{-}1)^{\mathrm{th}}$ order terms in order to obtain all the missing subtraction terms. The repeated procedure is somewhat lengthy and is thus presented in the Appendix A of this paper.

Note that the subtraction term from Equations 2.8,2.9 can be combined with either of the two hard cross-sections; joining it with $(\mathrm{n}\text{-}1)^{\mathrm{th}}$ (Eq. 2.4) order cross-section instead of n^{th} (Eq. 2.6) one gets:

$$\bar{\sigma}^{(n-1)}_{\mathrm{AB}\to\mathrm{X}} = (f_{H/A} - f_{g/A} \otimes f^{(1)}_{H/g}) \otimes \hat{\sigma}^{(n-1)}_{\mathrm{Hs}\to\mathrm{X}} \otimes f_{s/B} = \bar{f}_{H/A} \otimes \hat{\sigma}^{(n-1)}_{\mathrm{Hs}\to\mathrm{X}} \otimes f_{s/B} \ , \tag{2.11}$$

where the new parton distribution function $\bar{f}_{H/A} = (f_{H/A} - f_{g/A} \otimes f^{(1)}_{H/g})$ nicely expresses the physical origin of the subtraction term. In addition to being the collinear limit of the n^{th} order calculation, it also represents the first (fixed) order component of the QCD evolved parton distribution functions which is thus explicitly removed from the fully re-summed (to all orders in $\alpha_s \ln(\mu^2/m_H^2)$) function $f_{H/A}$.

The experimentalists are generally interested in the fully differential cross-sections from which exclusive topologies (events) can be picked. The procedure to obtain an exclusive topology from an inclusive differential cross-section is well established in various flavors [4, 5, 19] and is commonly known as the Sudakov parton showering. Using the case of Eq. 2.4 as an example, the Factorization Theorem states that the incoming heavy quark is fully resolved at the factorization scale $\mu = \mu_F$. The probability $d\mathrm{P}_{g\to H\bar{H}}(\mu)$ of the heavy quark un-resolving back to the gluon (back-evolution) at a lower scale $\mu < \mu_F$ (and producing an exclusive state with an additional $\bar{H}$) is then given by the differential of the Sudakov exponent (see e.g. [5]):

$$S_c = \exp\left\{ -\int\limits_{\mu^2}^{\mu_F^2} \frac{d\mu'^2}{\mu'^2} \frac{\alpha_s(\mu'^2)}{2\pi} \times \sum_a \int\limits_{\xi_c}^{1} \frac{dz}{z} P_{a\to c}(z) \frac{f_{a/I}(\frac{\xi_c}{z}, \mu'^2)}{f_{c/I}(\xi_c, \mu'^2)} \right\}. \tag{2.12}$$

$$dS_c(\mu) = \sum_a dS_{a\to c}(\mu) = \sum_a \frac{d\mu^2}{\mu^2} \frac{\alpha_s(\mu^2)}{2\pi} \frac{dz}{z} P_{a\to c}(z) \frac{f_{a/I}(\frac{\xi_c}{z}, \mu^2)}{f_{c/I}(\xi_c, \mu^2)} \times S_c$$

For the given example of gluon splitting to heavy quarks with $d\mathrm{P}_{g\to H\bar{H}}(\mu) = dS_{g\to H}(\mu)$ one gets:

$$d\sigma^{\mathrm{shower}}_{\mathrm{AB}\to\mathrm{X}\bar{\mathrm{H}}} = dS_{g\to H}(\mu)\, f_{H/A}(\mu_F)\, d\hat{\sigma}^{(n-1)}_{\mathrm{Hs}\to\mathrm{X}}\, f_{s/B}(\mu_F) \ , \tag{2.13}$$

which is also written as fully differential in all variables. Note that the $dS_{g\to H}(\mu)$ term in the Monte-Carlo context represents an explicit showering step (i.e. a parton-showered parton level 'hard' event). A fact also worth noting is that this expression is now of the order n and contains one resolved particle $\bar{H}$, thus giving the same configuration as the perturbative n^{th} order expression of Eq. 2.6 in the region $(\mu < \mu_F)$. There is clearly an overlap between the results of the two in this region, producing the 'double-counting' in the

overlap region. The subtraction term of Eq. 2.9 however retains its role also in differential form:

$$d\sigma^{(n)}_{\rm subt} = df^{(1)}_{H/g}(\mu)\, d\hat{\sigma}^{(n-1)}_{\rm Hs\to X} \qquad (\mu < \mu_F) \tag{2.14}$$

and this fully differential subtraction term depends on the variable μ through:

$$df^{(1)}_{H/g}(\mu) \;=\; \frac{\alpha_s(\mu_F)}{2\pi} P_{g\to H}(z) \frac{dz}{z} \frac{d\mu^2}{\mu^2}, \tag{2.15}$$

where the μ variable needs to be explicitly kinematically related to the mass singularity in the (differential) $\mathrm{n}^{\rm th}$ order cross-section. The Equation 2.6 can now be rewritten in differential form:

$$d\sigma^{(n)}_{\rm AB\to X\bar{H}} = f_{g/A}\, d\hat{\sigma}^{(n)}_{\rm gs\to X\bar{H}}\, f_{s/B} \;=\; f_{g/A}\, d\sigma^{(n)}_{\rm gs\to X\bar{H}}\, f_{s/B} \;-\; f_{g/A}\, d\sigma^{(n)}_{\rm subt}\, f_{s/B}\,. \tag{2.16}$$

Correspondingly, anticipating the exclusive final state containing one heavy quark, the differential form of Equation 2.8 is then given by:

$$\begin{aligned} d\sigma_{\rm AB\to X\bar{H}} \;=&\; f_{g/A}\, d\sigma^{(n)}_{\rm gs\to X\bar{H}}\, f_{s/B} \\ -&\; f_{g/A}\, d\sigma^{(n)}_{\rm subt}\, f_{s/B} \\ +&\; d\sigma^{\rm shower}_{\rm AB\to X\bar{H}}\,, \qquad\qquad (\mu < \mu_F) \end{aligned} \tag{2.17}$$

which, when inserting the explicit expressions from Equations 2.13 and 2.14 gives:

$$\begin{aligned} d\sigma_{\rm AB\to X\bar{H}} \;=&\; f_{g/A}(\mu_F)\, d\sigma^{(n)}_{\rm gs\to X\bar{H}}\, f_{s/B}(\mu_F) \\ -&\; f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu)\, d\hat{\sigma}^{(n-1)}_{\rm Hs\to X}\, f_{s/B}(\mu_F) \qquad\qquad (\mu < \mu_F) \\ +&\; dS_{g\to H}(\mu)\, f_{H/A}(\mu_F)\, d\hat{\sigma}^{(n-1)}_{\rm Hs\to X}\, f_{s/B}(\mu_F)\,. \qquad (\mu < \mu_F) \end{aligned} \tag{2.18}$$

It is trivially obvious that the subtraction term still cancels the collinear limit (mass divergence) of the perturbative $\mathrm{n}^{\rm th}$ order calculation of Eq. 2.16, while its impact on the $(\mathrm{n}\text{-}1)^{\rm th}$ order (showered) calculation is again best seen by combining the last two lines of Equation 2.18 and results of Eqns. 2.13 and 2.14 into:

$$d\bar{\sigma}^{(n-1)}_{\rm AB\to X\bar{H}} = \Big(dS_{g\to H}(\mu)\, f_{H/A}(\mu_F) \,-\, f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu)\Big)\, d\hat{\sigma}^{(n-1)}_{\rm Hs\to X}\, f_{s/B}(\mu_F)\,. \tag{2.19}$$

Taking the limit $\mu \to \mu_F$ one quickly sees that:

$$dS_{g\to H}(\mu)\, f_{H/A}(\mu_F) \;\xrightarrow{\mu\,\to\,\mu_F}\; f_{g/A}(\mu_F)\, \frac{\alpha_s(\mu_F)}{2\pi} P_{g\to H}\, d\Phi \tag{2.20}$$

$$f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu) \;\xrightarrow{\mu\,\to\,\mu_F}\; f_{g/A}(\mu_F)\, \frac{\alpha_s(\mu_F)}{2\pi} P_{g\to H}\, d\Phi, \tag{2.21}$$

with $d\Phi$ denoting all the variables in the differential. In this limit $\mu \to \mu_F$ the two terms thus cancel *on paper*, i.e. exactly. Since μ_F is by definition the highest virtuality reachable by parton showering approach, the kinematic region $\mu > \mu_F$ is thus populated solely by the $\mathrm{n}^{\rm th}$ order contribution and the continuation on the transition point is *smooth.* Choosing a kinematic relation which defines μ in terms of kinematic quantities measuring

the collinearity (e.g. transverse momentum of the splitting, virtuality of the participating particle/propagator) one achieves an ordered subtraction scheme ranging from the collinear region to the showering limit μ_F.

The result of these deliberations is that the subtraction term besides it's obvious role actually *smoothly interpolates* between the parton-shower evolved (n-1)$^{\text{th}}$ order and n$^{\text{th}}$ order perturbative expressions while removing the double-counting contributions in the overlap region ($\mu \leq \mu_F$).

There is no obvious reason why this procedure cannot be made iterative since the subtraction terms are designed to cancel all mass divergences present in a perturbative calculation of a certain order. In fact, a consistent iterative (and recursive) procedure has been developed and implemented in our paper [14], however the iterative nature of it was not tested in the examples developed thus far. The process of the associated Z boson production with two heavy (b) quarks $gg \to Z^0/\gamma b\bar{b}$ serves as a good test case when one wants both b-quarks to be resolved (observable) and correctly described over the whole phase space.

2.2 The Implementation of the Showering and Overlap Removal

In order to implement the above procedure in a Monte Carlo algorithm one needs to define a specific mapping of the variables μ, z in the Sudakov (parton) showering algorithm (c.f. Equation 2.13) as well as appropriate kinematic transforms between the four-momenta of the partons undergoing the showering.

The choice of the kinematic mappings and transforms to suit our procedure is in principle arbitrary, as long as it properly takes into account the heavy parton masses. Consequently the defined procedure could be matched to the parton showers of e.g. Pythia [5] or Herwig [19] if the mass of the partons were incorporated.

Nevertheless, we chose to implement our own showering algorithm based on the one suggested by Collins *et al* [11, 20, 21, 22] and extended it to properly incorporate heavy parton masses. The explicit derivation of the showering algorithm, kinematic mappings and transforms applied to our procedure have already been described in our previous paper [14]. Summarized briefly, the implemented showering algorithm has the evolution variable μ chosen to be equal to the virtuality of the particle (in our case heavy quark) and in each showering step the rapidity of the showered system is preserved, which sets the variable z of Equation 2.12. The value of the factorization scale μ_F is not pre-determined (i.e. can be picked from one of reasonable options, e.g. the invariant mass of the subsystem or similar).

The choice of the showering algorithm implementation was motivated by two main points:

- This subtraction term of Equation 2.14, albeit derived in a different way, is in form identical to the subtraction term derived by Collins *et al.* This fact motivated us to implement the parton showering algorithm according to prescriptions given in the cited papers.

- The selected kinematic setup is motivated by the fact that, as shown by Collins *et al* [11, 20, 21, 22], the procedure of parton showering and subtraction is not equivalent to

the standard subtraction schemes (e.g. $\overline{\mathrm{MS}}$) and thus the parton distribution functions should in principle be modified. The modification is generally non-trivial (using e.g. Pythia [5] showers), however using this specific choice of showering kinematics the corrected (JCC) scheme is for quarks simply related to the $\overline{\mathrm{MS}}$ parton distribution functions:

$$\begin{aligned} z\, f^{\mathrm{JCC}}_{i/I}(z,\mu^2) &= z\, f^{\overline{\mathrm{MS}}}_{i/I}(z,\mu^2) \\ &+ \frac{\alpha_s(\mu^2)}{2\pi}\int_z^1 d\xi \frac{z}{\xi} f^{\overline{\mathrm{MS}}}_{g/I}(\xi,\mu^2)\left[P_{g\to i}(\frac{z}{\xi})\ln\left(1-\frac{z}{\xi}\right)+\frac{z}{\xi}\left(1-\frac{z}{\xi}\right)\right] \\ &+ \mathcal{O}(\text{first-order quark terms}) \; + \mathcal{O}(\alpha_s^2)\,. \end{aligned} \tag{2.22}$$

The above Equation 2.23 does not apply to gluons. It needs to be pointed out that at present it is not known how to simply extend this approach to gluons. For the interested reader on the work in this direction we recommend the paper [29].

It needs to be emphasised that for the purpose of this paper, only a very narrow implementation of the showering algorithm was needed, namely a single heavy quark backward branching to gluon and subsequently only this part was actually implemented in place of a full parton showering program.

We can now summarize the properties of thus obtained algorithm of combining pQCD and parton showering as implemented in our Monte-Carlo algorithm:

- All heavy quarks (incoming and outgoing) are kept *massive* throughout the procedure, both in the perturbative calculation of matrix elements and in the showering procedure and overlap removal. The matrix elements used are at present 'leading order' (tree-level) only, however the procedure could in principle be expanded to diagrams containing virtual corrections.

- All overlap removal is done at the parton level on an event-by-event basis. The collinear topologies are determined from the participating Feynman diagrams (currently done manually but could in theory be automatized).

- The kinematics of the shower and overlap removal is implemented especially for this approach. These choices are reflected in the subtraction term which is achieved by calculating the collinear limit of the kinematic topology (event) of the n$^{\mathrm{th}}$ order perturbative calculation.

The event generation is thus performed in the following steps:

- The n$^{\mathrm{th}}$ order process (event) is sampled, the collinear limits for the given event topology are estimated and the subtraction terms of order (n-1) are calculated. The weight is given by Equation 2.16.

- The (n-1)$^{\mathrm{th}}$ order process (event) is sampled. If this process still contains gluon splitting to heavy quarks in the initial state (in the other incoming leg) the corresponding subtraction terms of order (n-2) are again calculated. The event is then showered and the weight is given by Equation 2.13.

- If subtraction terms were found in the previous step, the corresponding (n-2)$^{\mathrm{th}}$ order process is calculated and showered on both legs to achieve the (n$^{\mathrm{th}}$ order) event configuration of the previous two cases. The weight is estimated analogous to Equation 2.13 for two showering steps.

All the above classes of events are separately unweighted, obtaining weights equal to ± 1 because in some phase space points the contributions from subtraction terms can actually be greater than the unsubtracted values, as will be shown in the following sections. The summed contributions of all processes, corresponding to Equation 2.17, are of course positive throughout the phase space. In the actual Monte-Carlo program, it is very easy to (pre-)mix these classes of events internally to obtain the summed contribution corresponding to Equation 2.17.

The procedure of [14] has been improved by introducing the *massive* splitting kernel correction for the initial state $g \to H\bar{H}$ splits, which can be derived from [23] results:

$$P^{\mathrm{massive}}_{g\to H} = P^{\mathrm{massless}}_{g\to H} + P^{\mathrm{correction}}_{g\to H} = \mathrm{T_R}\ (1-2z(1-z)) + \mathrm{T_R}\left(\frac{2z(1-z)m_H^2}{p_T^2+m_H^2}\right), \qquad (2.23)$$

with p_T being the relative transverse momentum of the spectator heavy quark in the split. The massive kernels have already been used for final state showering in the Sherpa Monte-Carlo generator [4] but have to our knowledge never been used in the showering of initial state heavy quarks.

2.3 The $gg \to Z^0/\gamma^* b\bar{b} \to f\bar{f}b\bar{b}$ Implementation

Assuming an experimentalist at LHC wants to study the Drell-Yan production with two resolved (heavy) b-quarks in the final state, one now has three possible choices of calculation (c.f. Figure 3):

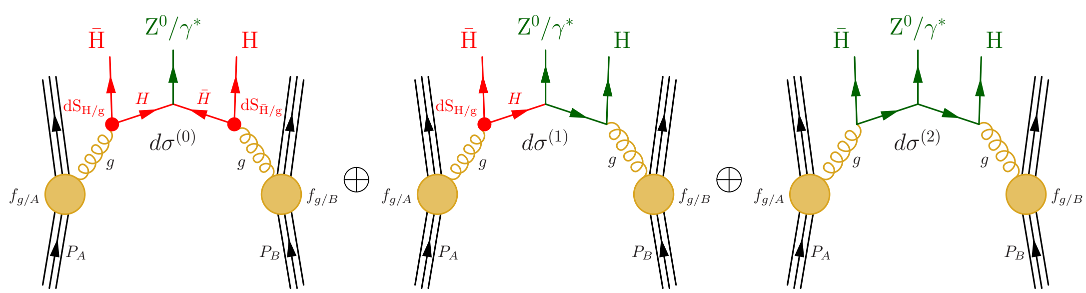

Figure 3: Schematic representation of contributions resulting in exclusive $Z^0 H\bar{H}$ final state: two fully evolved heavy (b) quarks entering 'pure' Drell-Yan at order α_s^0 in combination with double initial state parton shower (left), one heavy quark and one gluon entering the hard process at order α_s^1 in combination with one parton shower (middle) and fully perturbative calculation involving two incoming gluons in a hard process of order α_s^2 (right). These three processes need to be combined with appropriate overlap removal as detailed in the text.

- The order α_s^0 hard process $b\bar{b} \to Z^0/\gamma^* \to f\bar{f}$ with fully evolved b-quarks entering the hard process at μ_F. The cross-section contains no mass singularities and needs

no subtraction terms ($d\hat{\sigma}^{(0)} = d\sigma^{(0)}$). The associated b-quarks are then resolved at scales μ_{1H} and $\mu_{2\bar{H}}$ using parton showering:

$$d\sigma^0_{AB\to Z^0/\gamma^* b\bar{b}} = \sum_{H=b,\bar{b}} dS_{g\to H}(\mu_{1H})\, f_{H/A}(\mu_F)\, d\sigma^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}}\, dS_{g\to \bar{H}}(\mu_{2\bar{H}})\, f_{\bar{H}/B}(\mu_F)\ . \tag{2.24}$$

Kinematically, the leg with higher induced virtuality (scale) is treated (unresolved to gluon) first.

- The order α_s^1 hard process $gH \to Z^0/\gamma^* \to f\bar{f}\ H$, $H = b, \bar{b}$ with one fully evolved b-quark entering the hard process at μ_F and the other one participating as the propagator inside the matrix element calculation. The cross-section thus contains one mass singularity related to the propagator and needs a subtraction term derived from the collinear limit of the b-quark propagator. The other associated b-quark is then resolved using parton showering and the scales $\mu_{1,2}$ are set to be the evolution scale of the showered quark and the virtuality of the b-quark propagator respectively:

$$\begin{aligned} d\sigma^1_{AB\to Z^0/\gamma^* b\bar{b}} &= \sum_{H=b,\bar{b}} dS_{g\to H}(\mu_{1H})\, f_{H/A}(\mu_F)\, d\sigma^{(1)}_{\mathrm{Hg\to Z^0/\gamma^*\, H}}\, f_{g/B}(\mu_F) \\ &+ \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, d\sigma^{(1)}_{\mathrm{g\bar{H}\to Z^0/\gamma^*\, \bar{H}}}\, dS_{g\to \bar{H}}(\mu_{2\bar{H}})\, f_{\bar{H}/B}(\mu_F) \\ &- \sum_{H=b,\bar{b}} dS_{g\to H}(\mu_{1H})\, f_{H/A}(\mu_F)\, d\sigma^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}}\, df^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\, f_{g/B}(\mu_F) \\ &- \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu_{1H})\, d\sigma^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}}\, dS_{g\to \bar{H}}(\mu_{2\bar{H}})\, f_{\bar{H}/B}(\mu_F)\ . \end{aligned} \tag{2.25}$$

- The order α_s^2 hard process $gg \to Z^0/\gamma^* b\bar{b} \to f\bar{f}b\bar{b}$ where both incoming b-quarks participate as propagators inside the matrix element calculation. The cross-section thus contains two mass singularities related to the propagators and needs corresponding subtraction terms (with permutations) derived from the collinear limit of the two b-quark propagators, virtualities of which then define the scales $\mu_{1,2}$. Using the formalism of [14], or equivalently [9], one obtains:

$$\begin{aligned} d\sigma^2_{AB\to Z^0/\gamma^* b\bar{b}} &= f_{g/A}(\mu_F)\, d\sigma^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}}\ f_{g/B}(\mu_F) \\ &- \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu_{1H})\, d\sigma^{(1)}_{\mathrm{Hg\to Z^0/\gamma^*\, H}}\, f_{g/B}(\mu_F) \\ &- \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, d\sigma^{(1)}_{\mathrm{g\bar{H}\to Z^0/\gamma^*\, \bar{H}}}\, df^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\, f_{g/B}(\mu_F) \\ &+ \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, df^{(1)}_{H/g}(\mu_{1H})\, d\sigma^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}}\, df^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\, f_{g/B}(\mu_F)\ . \end{aligned} \tag{2.26}$$

The derivation of the above subtraction terms is presented in Appendix A.

One might be surprised at the + sign of the last 'subtraction' term in Eq. 2.26 however re-arranging the subtraction terms to be matched with the corresponding showering

expressions in the spirit of Eq. 2.19 one derives the tree cross-section differentials:

$$d\bar{\sigma}^0 = \sum_{H=b,\bar{b}} \Big(dS_{g\to H}(\mu_{1H})\, f_{H/A}(\mu_F) \,-\, df^{(1)}_{H/g}(\mu_{1H})\, f_{g/A}(\mu_F) \Big)\, d\sigma^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}} \times \\ \times \Big(dS_{g\to \bar{H}}(\mu_{2\bar{H}})\, f_{\bar{H}/B}(\mu_F) \,-\, df^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\, f_{g/B}(\mu_F) \Big) \tag{2.27}$$

$$d\bar{\sigma}^1 = \sum_{H=b,\bar{b}} \Big(dS_{g\to H}(\mu_{1H})\, f_{H/A}(\mu_F) \,-\, df^{(1)}_{H/g}(\mu_{1H})\, f_{g/A}(\mu_F) \Big)\, d\sigma^{(1)}_{\mathrm{Hg\to Z^0/\gamma^*\,H}}\, f_{g/B}(\mu_F) \\ + \sum_{H=b,\bar{b}} f_{g/A}(\mu_F)\, d\sigma^{(1)}_{\mathrm{g\bar{H}\to Z^0/\gamma^*\,\bar{H}}} \Big(dS_{g\to \bar{H}}(\mu_{2\bar{H}})\, f_{\bar{H}/B}(\mu_F) \,-\, df^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\, f_{g/B}(\mu_F) \Big) \tag{2.28}$$

and trivially:

$$d\bar{\sigma}^2 = f_{g/A}(\mu_F)\, d\sigma^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}}\;\, f_{g/B}(\mu_F)\,. \tag{2.29}$$

As noted above, there are actually four scales $\mu_{1H,2\bar{H}}, (H = b, \bar{b})$, namely the virtualities assuming that the b-quark (anti-quark) are connected to the first (second) gluon from hadrons A and B. From the above forms it is evident that the first contribution from Eq. 2.27 is zero when either of $\mu_{1,2} = \mu_F$ as are respective terms in Eq. 2.28, ensuring the smooth transitions of the functions in the region close to the factorization scale as expected. Subsequently, the behavior of the subtraction terms corresponds to four scenaria $\mu_{1,2} < \mu_F$ where all the tree contributions are non-zero, $\mu_1 < \mu_F, \mu_2 > \mu_F$ and $\mu_2 < \mu_F, \mu_1 > \mu_F$ where only the contributions from Eqns. 2.28 and 2.29 are non-zero and the region $\mu_{1,2} > \mu_F$ where only the fully perturbative contribution of Eq. 2.29 contributes. Graphically, the contributions are shown in Figure 4.

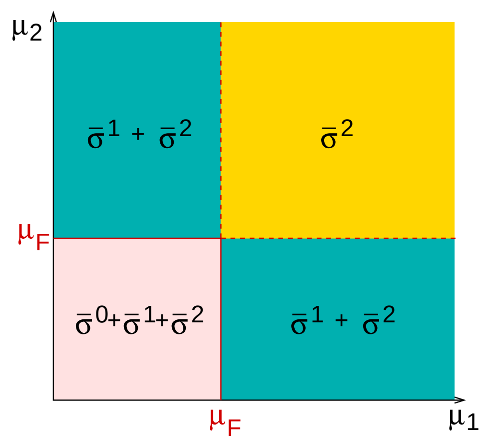

Figure 4: Schematic representation of contributions sources corresponding to four scenaria $\mu_{1,2} < \mu_F$ where all the tree contributions are non-zero, $\mu_1 < \mu_F, \mu_2 > \mu_F$ and $\mu_2 < \mu_F, \mu_1 > \mu_F$ where only the contributions from Eq. 2.28 and 2.29 are non-zero and the region $\mu_{1,2} > \mu_F$ where only the fully perturbative contribution of Eq. 2.29 contributes.

At this point one should also review the omissions (limitations) of the proposed algorithm: As presented in Equations 2.24-2.29 the terms $dS_{g\to H}(\mu)$ indicate that there is no emission between the scales $[\mu_{1,2}, \mu_F]$ (c.f. Eq. 2.13), i.e. the heavy quark unresolves (backward evolution) directly to gluon. All the tree contributions will thus uniquely produce the same initial (gg) and final ($\mathrm{Z^0/\gamma^*\, b\bar{b}}$) state.

In a full shower implementation as e.g. in Pythia [5], HERWIG [19] or Sherpa [4], one or more additional branchings in terms of gluon radiation H → gH could take place before the heavy quark would resolve back to a gluon via gluon splitting. Consequently,

a part of the contributions, which would be present in case of a full shower from inclusive $\mathrm{gH} \to \mathrm{Z}^0/\gamma^*\,\mathrm{H}$ and $\mathrm{H}\bar{\mathrm{H}} \to \mathrm{Z}^0/\gamma^*$ production, is missing. The probabilities of omitted showering contributions are however considered to be small, using again the argument of the order of heavy quark density $f_{H/I}$ being of the effective order α_s higher with respect to the gluon PDFs and considering the dS form of Eq. 2.13.

3. Implementation and Results

The process $gg \to Z^0/\gamma^* b\bar{b}$ is implemented in the AcerMC Monte-Carlo generator [3] using the (adapted) MadGraph [24] matrix elements with full Z^0/γ^* interference. Unweighted events corresponding to the three sub-processes, given by Equations 2.24, 2.25 and 2.26, are generated with native AcerMC single heavy quark backward branching to gluon [14]. Each dS term in the Eq. 2.24, 2.25 and 2.26 thus corresponds to an actual parton showering step in the event generation.

As already stated, only a very narrow implementation of the showering algorithm was needed for the purpose of this paper, namely a single heavy quark backward branching, and subsequently only this part was actually implemented in place of a full parton showering algorithm. The produced parton level events from AcerMC thus need to be passed to Monte Carlo tools as Pythia [5] or HERWIG [19] for further showering and hadronization.

The showering algorithms in AcerMC (implemented in the style of Pythia veto sampling) can in principle easily be expanded to full shower with both initial and final state radiation and all possible branchings but for purposes of this paper we only needed that single showering step. Although the implementation of the full showering in AcerMC would guarantee consistence by using only one showering algorithm (whereas now it needs to be extended with further Pythia or Herwig showers with different showering algorithms), the subsequent interface of the partons to the fragmentation algorithms in Pythia or Herwig would be rather difficult and beyond the scope of this project.

Due to the subtraction terms a fraction of event candidates achieve negative sampling weights and unweighted events are produced with weight values of ± 1 using the standard unweighting procedures. In the subsequent studies only the pure $Z^0 \to \mu^+\mu^-$ channels were used for benchmarking (the photon contribution was turned off) in the LHC environment (proton-proton collisions at $\sqrt{\mathrm{s}} = 14$ TeV) in combination with the CTEQ6L1 [25] and hence derived JCC PDF sets[1] to manifestly see the impact of using the JCC (Eq. 2.23) modification, which turns out to be sizable in the b-quark case, contrary to its impact on the light quark PDF values. Let us emphasize again that Collins *et al* have shown in [11, 20, 21, 22] that the PDF sets obtained e.g. in the $\overline{\mathrm{MS}}$ subtraction scheme as the CTEQ sets are not formally the correct ones to be used in parton showering but that instead modified PDF sets corresponding to the showering algorithm (as the JCC for the Collins-style shower prescription implemented in AcerMC) should be used. In other words,

[1]There is a possibly valid argument that the NLO PDF sets should be used instead of LO ones since the derived procedure is in part NLO. The choice of these does not affect our results qualitatively and affects above all the absolute normalization (cross-section) prediction which is not correct anyway due to the absence of virtual corrections to our calculations.

the PDFs in Monte-Carlo event generators are determined by the showering algorithm and cannot be freely chosen, unlike the case for PDFs used in inclusive calculations.

The b-quark mass is set to $m_b = 4.8$ GeV and the factorization and renormalization scales were chosen to be equal to the Z^0 mass ($\mu_F = M_Z$) but of course other choices are possible. All the presented results are at parton level (i.e. b-quarks, Z^0/γ^* and its decay products) as output by AcerMC.

It is instructive to first reproduce the order α_s^1 results derived in our paper [14] in order to check the impact of the massive evolution kernels introduced in this paper (Eq. 2.23). The results are presented in Figure 5.

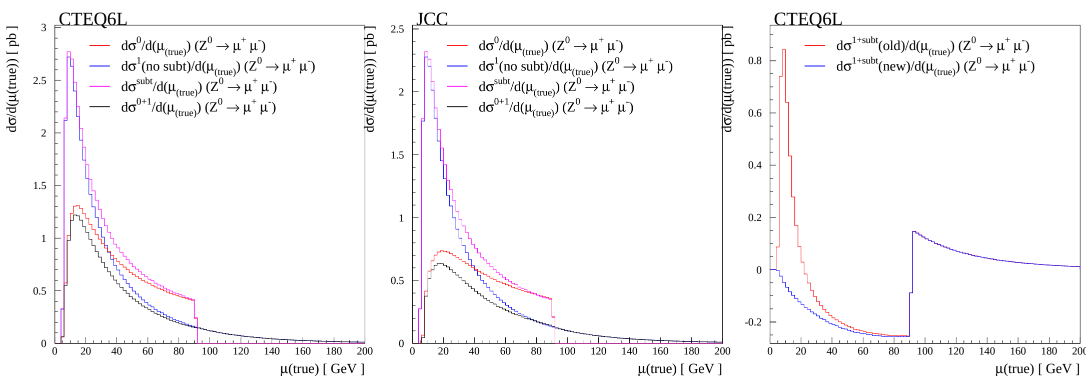

Figure 5: The reproduced order α_s^1 results from [14] using the CTEQ6L1 and JCC PDF sets (left and middle); note that the subtraction term (magenta line) indeed gives a smooth transition from low μ region, where it matches the perturbative calculation (blue) to the $\mu = \mu_F$ region where it matches the parton shower prediction (red). In the right plot the impact of introducing massive splitting kernels is shown explicitly for the order α_s^1 prediction combined with the subtraction term; note that the low μ peak previously present in [3] now disappears completely.

As one can observe in the rightmost plot of Fig. 5 the introduction of massive splitting kernels has corrected the low scale (virtuality) region; the subtraction term now indeed smoothly interpolates between the low scale (collinear limit) where it matches the order α_s^1 contribution to the factorization scale $\mu_F = M_Z$ where it coincides with the parton shower prediction as expected, thus allowing smooth transition between the two contributions as predicted. Note that at the order α_s^1 *two* virtualities for incoming b-quarks are picked from the Sudakov back-evolution (to gluon) of the order α_s^0 pure Drell-Yan process but only *one* leg is actually showered and correspondingly only one subtraction term is introduced in the order α_s^1 process. Since in this case there is no ambiguity one can trace the actual μ used in the shower evolution and subtraction (labeled μ(true) in Figure 5).

This is however not the case once we go to the full α_s^2 order where, as already stated, all the incoming b-quarks are showered back to gluons. Here four possible scale choices exist $\mu_{i=1,4} = -(p(g_{1,2}) - p(b,\bar{b}))^2 + m_b^2$ and multiple overlap removal terms can contribute. We thus chose to plot the virtualities/scales related to first gluon and b-quark (μ_1) and second gluon and anti-b quark (μ_2) and their combinations; all other permutations in computing

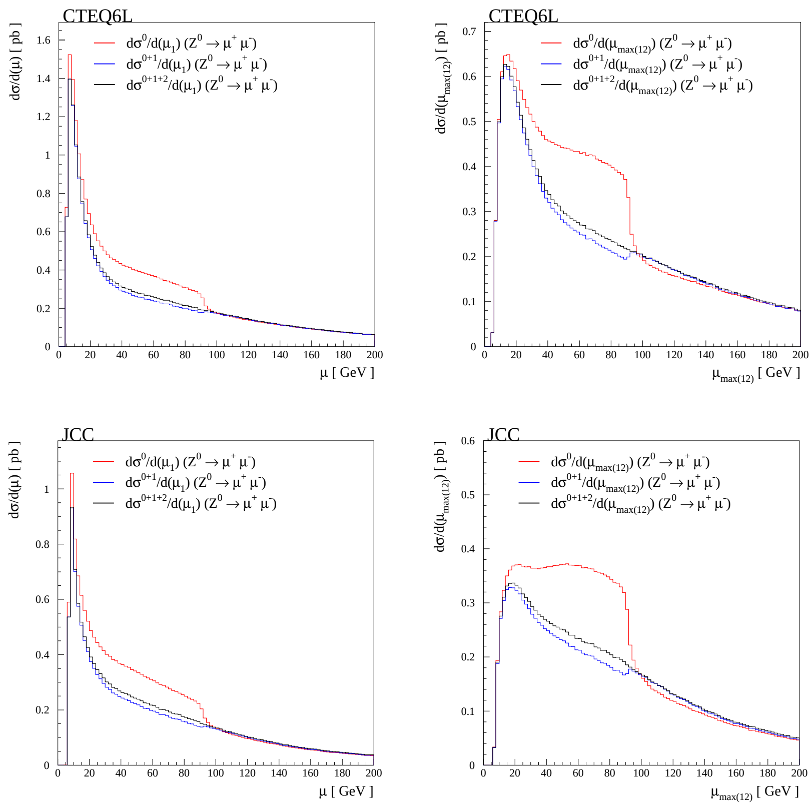

Figure 6: The full order α_s^2 results using the CTEQ6L1 (top) and JCC PDF sets (bottom), showing the distribution with respect to the virtuality/scale related to first gluon and b-quark (μ_1) (left) and maximal value of μ_1 μ_2 (virtuality/scale of the second gluon and anti-b quark) (right). As predicted the summed contribution with overlap removal gives a smooth distribution despite the sharp cutoff at $\mu = \mu_F = M_Z$.

the virtualities give identical predictions. The one-dimensional plots, as presented in Figure 6, again confirm the predictions of our approach resulting in a smooth distribution from the combination of different order contributions. The contributions to the total cross-sections are given in Table 1.

One can observe that the contribution of the order α_s^2 is small both in the absolute normalization and its contribution to the one-dimensional projections. Its impact and importance is better observable plotting the two dimensional (μ_1, μ_2) differential cross-section plots presented in Figures 7,8. Apart from contributing to its 'exclusive' region of high $\mu_{1,2} >> \mu_F$ it contains a significant correction in the region $\mu_1 \simeq \mu_2$ throughout the $\mu_{1,2}$ value range. Upon reflection this is to be expected since the perturbative-level calculation (and thus the full combined result) should not be biased around the $\mu_1 \simeq \mu_2$ region whereas the parton-showering approach by definition *is biased* in this region, especially at values close to μ_F. The probability of having *both* $\mu_{1,2}$ large is the square of probability to obtain a single large μ value and its value is thus supposed to be low, with the observable dip in the $\mu_{1,2}$ distributions Figures 7,8 which the order α_s^2 contribution fills

Process	$\sigma_{\mathrm{CTEQ6L1},\mu_{\mathrm{F}}=\mathrm{m_Z}}$ [pb]	$\sigma_{\mathrm{JCC},\mu_{\mathrm{F}}=\mathrm{m_Z}}$ [pb]
σ^0	64.4	44.8
σ^1	-10.7	-8.9
σ^2	2.0	2.0
$\Sigma_i \sigma^i$	55.7	37.9
$gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$	22.9	22.9

Table 1: The process cross-sections for the leading order α_s^0 contribution integrated cross-section σ^0, order α_s^1 contribution σ^1 including the subtraction terms and order α_s^2 contribution σ^2, also with full overlap removal, are shown for the $Z^0 \to \mu^+\mu^-$ decay channel in the LHC environment (proton-proton collisions at $\sqrt{\mathrm{s}} = 14$ TeV) are listed. The b-quark mass is set to $m_b = 4.8$ GeV and the factorization and renormalization scales are set to the Z^0 invariant mass squared. In addition, the perturbative (order α_s^2) $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process cross-section is shown for comparison. The cross-sections are given for the LO CTEQ6L1 [25] and the derived JCC PDFs. In the Monte-Carlo event generation procedure the next-to-leading process weights are combined with the subtraction weights on the event-by-event basis as described in the text.

up as expected.

The kinematic quantity of interest is also the impact of subsequent corrections on the transverse momentum of the Z^0 boson and b-quarks as shown in the Figure 9. Again, the order α_s^2 contribution seems to be comparatively small but is of importance in the very high transverse momentum regions. As it might be, one needs the full order α_s^2 procedure to achieve the exclusive final state containing two b-quarks and formally obtain the full symmetry in the procedure.

4. Conclusions and Further Perspective

It is instructive to compare our procedure to the procedure developed in the MC@NLO [26] framework. The MC@NLO Monte-Carlo generator incorporates an approach which results in double-counting removal both in the initial and final state — using massless quarks in the initial state — at full NLO, including virtual corrections, while our approach is currently developed to use only tree-level matrix elements but can be used iteratively to at least α_s^2 as shown in the given paper. Still, for our approach to be consistent, it should be compatible to the MC@NLO formalism and it will be shown this is indeed the case. MC@NLO is in its formalism following the paradigm of 'minimal intrusion' into the (showering) Monte-Carlo and is being interfaced to HERWIG Monte-Carlo generator [19] with the kinematic translations adapted to its showering (evolution parameters etc ...). Fortunately, it turns out one does not need to go into details to show the consistency of the two approaches; it is enough to use the 'master modified subtraction equation' of the

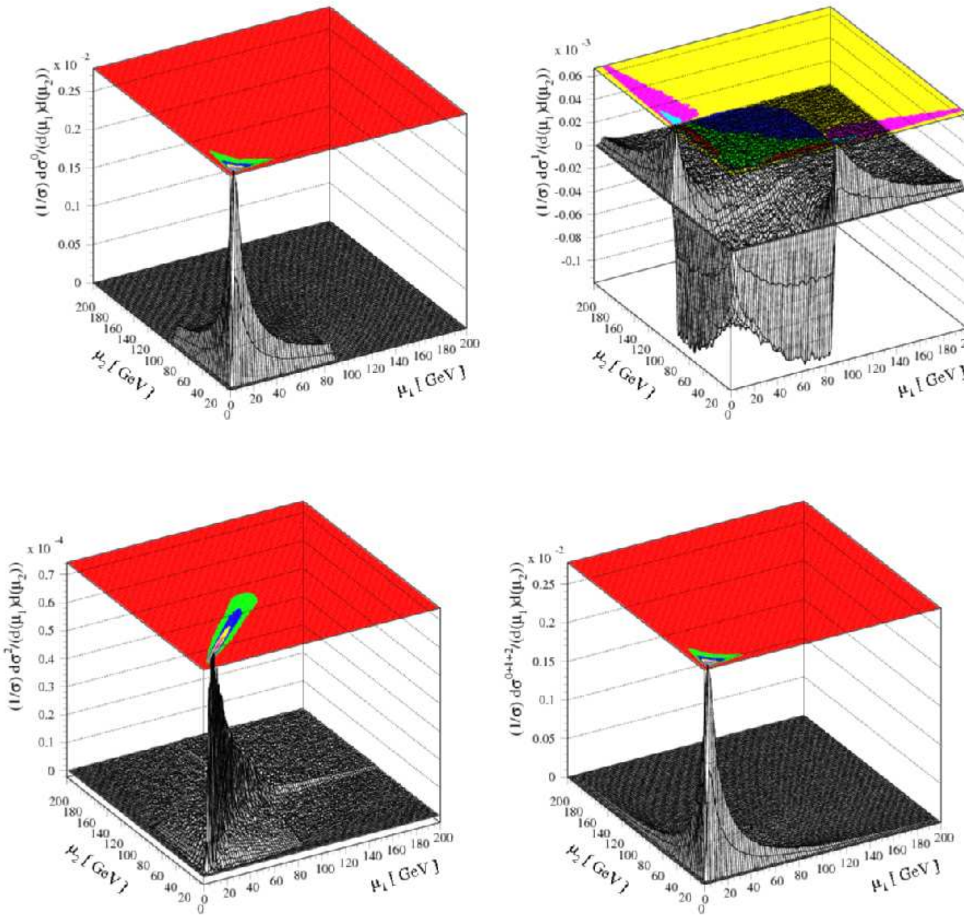

Figure 7: The full order α_s^2 results using the JCC PDF sets, showing the (normalized) distributions with respect to the virtuality/scale related to first gluon and b-quark (μ_1) and virtuality/scale of the second gluon and anti-b quark) (μ_2) for separate contributions including their subtraction terms. On the bottom right the sum of all contributions is shown to give a smooth distribution over the whole region as expected.

MC@NLO toy model in [26], i.e. Equation (3.20), which states:

$$\left(\frac{d\sigma}{dO}\right)_{\text{msub}} = \int_0^1 dx \Bigg[I_{\text{MC}}(0, x_M(x)) \frac{a[R(x) - BQ(x)]}{x} + I_{\text{MC}}(0,1)\left(B + aV + \frac{aB[Q(x)-1]}{x}\right)\Bigg], \tag{4.1}$$

where B represents the LO Born term, aV the finite part of the virtual corrections, $aR(x)/x$ the unsubtracted real corrections and $Q(x)$ is the Sudakov evolution kernel. The MC 'term',

$$I_{\text{MC}}(0, x_M)\frac{aBQ(x)}{x}, \tag{4.2}$$

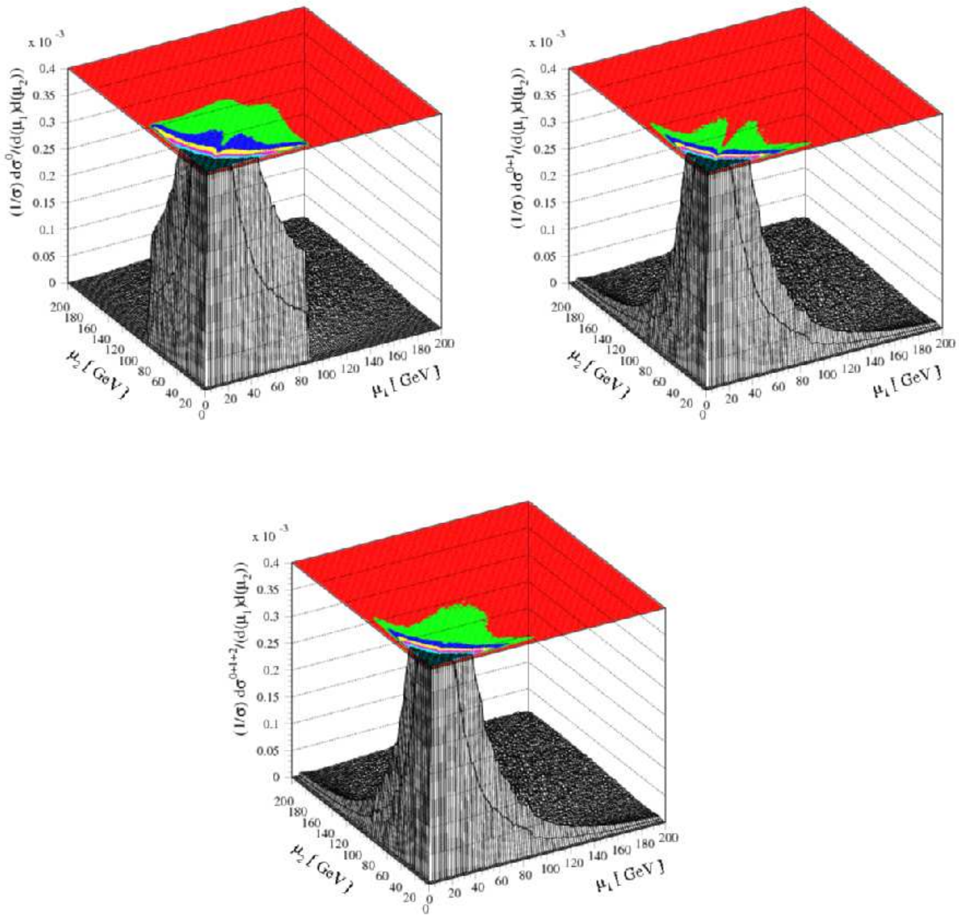

Figure 8: The full order α_s^2 results using the JCC PDF sets, showing the (normalized) distributions with respect to the virtuality/scale related to first gluon and b-quark (μ_1) and virtuality/scale of the second gluon and anti-b quark) (μ_2) for gradual combinations of contributions of order $\alpha_s^{0,1,2}$ including their subtraction terms. Note especially the disappearance of the dip in the region $\mu_1 \simeq \mu_2$ as detailed in the text.

equivalent to our subtraction terms, is in the above case *both subtracted and added* to the NLO cross-section expression to obtain two separately finite contributions. As stated, in MC@NLO the shower evolution is assumed fixed/pre-defined by the Monte Carlo program (defining the x as evolution variable and $Q(x)$ as the showering kernel) while the subtraction scheme at NLO, which removes the divergences and defines its own subtraction kernels is chosen separately (e.g. $\overline{\text{MS}}$). For simplicity in the MC@NLO toy model the subtraction kernel is set simply to one and the numerator $aB[Q(x)-1]$ in last fraction in Eq. 4.1 represents precisely the difference between the shower evolution kernel (scheme) and the NLO subtraction kernel (scheme).

If one instead chooses another approach and *adjusts* the shower and NLO subtraction

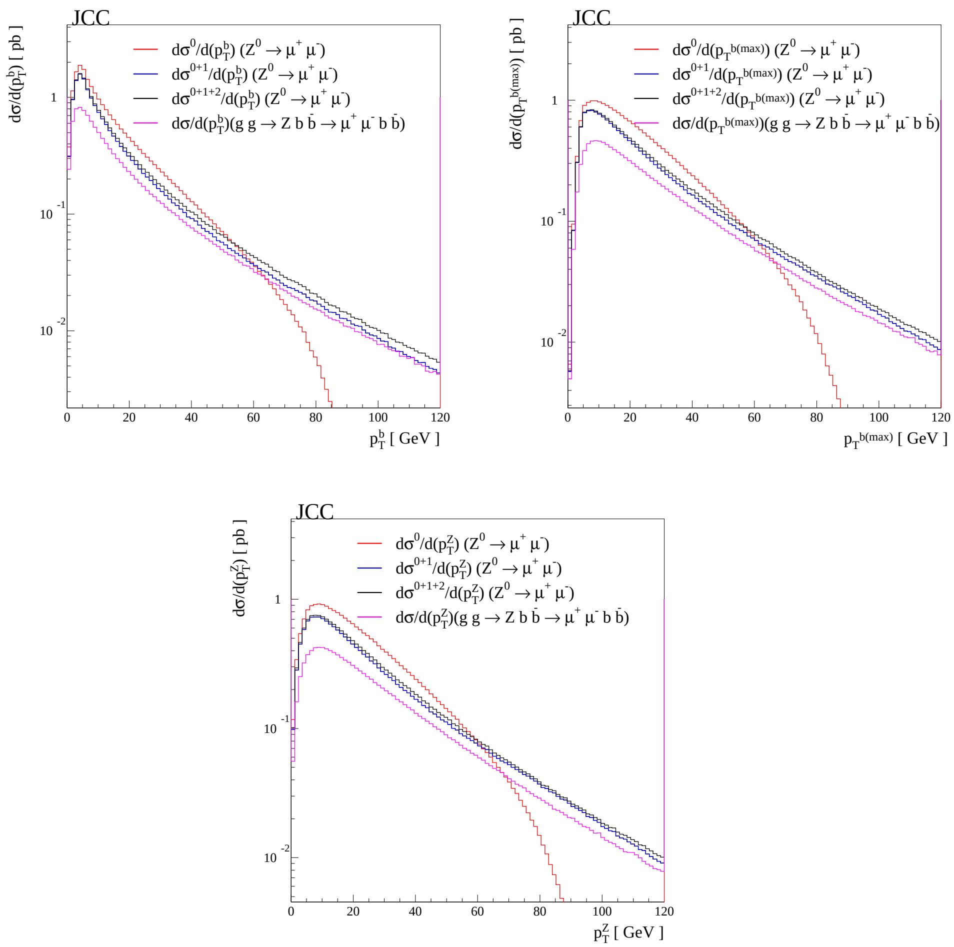

Figure 9: The full order α_s^2 results using the JCC PDF sets, showing the differential cross-sections with respect to the b-quark transverse momentum (left), maximal b-quark transverse momentum (middle) and Z boson transverse momentum (right). The perturbative calculation of order α_s^2 without subtractions is shown separately for comparison (magenta line).

schemes to match, i.e.

$$[Q(x) - 1] \to [Q_{\text{shower}} - Q_{\text{NLO}}] \to 0, \tag{4.3}$$

one gets instead:

$$\begin{aligned}\left(\frac{d\bar{\sigma}}{dO}\right)_{\text{msub}} = \int_0^1 dx \Big[& I_{\text{MC}}(0, x_M(x)) \frac{a[R(x) - BQ(x)]}{x} \\ & + I_{\text{MC}}(0,1)\,(B + aV\,)\Big],\end{aligned} \tag{4.4}$$

where the MC term is present only in subtraction from the real contribution but the NLO subtraction scheme is *re-defined* to match the showering scheme. If one disregards the finite virtual correction (which affects only the normalization) and particle masses this matches

exactly the formula of our approach. It also becomes clear that the parton distribution functions need to be re-defined since we are no longer in the $\overline{\mathrm{MS}}$ scheme (or any other standard scheme) but in a shower-governed scheme as clearly explained by Collins *et al* [21, 22].

The above comparison also shows the current limits of this approach: Our method assumes that there are no other divergent terms in the cross-sections apart from the mass divergences; furthermore, the expressions for shower scheme JCC parton distribution functions have so far been developed only for quarks. Consequently, if one wants to incorporate the presence of e.g. gluon radiation/splits in the hard process this approach would need to be extended, combined with other approaches (e.g. the addition of light 'jet-objects' through an algorithm like Vincia [27] or dipole showers [28]) or possibly even take new directions [29]. Nevertheless, facing the stated limitations, the presented procedure is thus shown to be consistent with MC@NLO approach at NLO order (α_s^1 corrections), while it does not include virtual (normalization) corrections.

Another point of interest is to compare our approach to the one of L-CKKW [12],[30] as the most advanced parton shower and matrix element matching algorithm so far. While L-CKKW defines a very sophisticated interpolation scheme it only picks the *dominant* collinear topology on an event-by-event basis by virtue of the employed jet clustering; in contrast, in our approach more than one collinearity can be accounted for and subtracted for each event. Furthermore, L-CKKW, while removing the double counting, was not (yet) shown to be formally correct in case of hadrons as the colliding particles [31]. On the other hand, the procedure described in this paper currently works only for initial state splits involving heavy quarks; in multi-particle final states the heavy quark lines are generally expected to be comparatively few. This would lead to a very complex procedure if light quarks/gluons were added, while it might not be necessary from the practical perspective since L-CKKW seems to be describing the multi-light-jet final states very well and could probably also be combined as a continuation of the procedure presented in this paper.

The near-future plans are to extend this approach to the heavy quark production in the final state gluon splits $g \to H\bar{H}$ and to implement the same formalism in the associated $Hb\bar{b}$ production which does in itself not need any further development of the formalism. There are certainly also plans to compare our approach with other $gg \to Z^0/\gamma^* b\bar{b}$ implementations and its impact to the LHC predictions is certainly envisaged but requires further work at the level of mock experimental LHC analysis and is thus digressing from the scope of the current paper.

A. Derivation of the Hard Cross Section Expressions and Subtraction Terms

The hard cross-section expressions and corresponding subtraction terms can according to [9] be actually be derived from the Factorization Theorem itself by using the Factorization Theorem *at the parton level* and doing power counting of α_s. Specifically, at a given order in α_s^n the factorization Theorem implies that the perturbative pQCD cross section $\sigma^{(\mathrm{n})}_{\mathrm{ab}\to\mathrm{X}}$ involving initial state partons a, b is related to its corresponding *hard* cross section $\hat{\sigma}^{(\mathrm{n})}_{\mathrm{ab}\to\mathrm{X}}$

(containing no mass singularities and being completely infra-red safe) by the modified Factorization Theorem[2]:

$$\sigma^{(n)}_{ab\to X} = \sum_{c,d} f^{(n_1)}_{c/a} \otimes \hat{\sigma}^{(n_2)}_{cd\to X} \otimes f^{(n_3)}_{d/b}, \tag{A.1}$$

where the sum of n_i terms gives the correct order n, i.e. $n = n_1 + n_2 + n_3$. The above equation differs from the regular Factorization Theorem expression in two respects:

- The parton distributions are in this case relative to an on-shell *parton* target.
- These parton-level distributions are expanded in powers of α_s, with $f^{(n_1)}_{c/a}$ denoting the term of order $\alpha_s^{n_1}$ in the distribution function expansion.

Furthermore, we limit ourselves to the case where at least one of the evolved incoming partons c, d is massive with mass M_H. Using the ACOT scheme [7, 8], the above parton densities are calculated in the $\overline{\text{MS}}$ scheme in the region $\mu > M_H$ at the first two orders in α_s as:

$$f^{(0)}_{j/i}(\xi) = \delta^j_i \delta(\xi - 1) \tag{A.2}$$

$$f^{(1)}_{H/i}(\xi,\mu) = \frac{\alpha_s(\mu)}{2\pi} P_{i\to H}(\xi) \ln\left(\frac{\mu^2}{m_H^2}\right), \tag{A.3}$$

$$f^{(1)}_{g/g}(\xi,\mu) = \frac{\alpha_s(\mu)}{2\pi} \delta(\xi - 1) \ln\left(\frac{\mu^2}{m_H^2}\right), \tag{A.4}$$

where $i, j = \{g, H\}$ and $P_{i\to H}(\xi)$ are the (usual) first order splitting kernels for (heavy) quark production. In addition, in this scheme, the pQCD cross-section $\sigma^{(n)}_{ab\to X}$ should already have been regularized using the $\overline{\text{MS}}$ scheme and the collinear singularities should have already been subtracted resulting in a finite cross section with only the mass singularities (meaning, at finite M_H, large logarithms $\ln(\mu^2/m_H^2)$) still present. In the calculation the light quark masses should be set to zero and the M_H kept at non-zero value throughout the calculation (contrary to the conventional approach where M_H is eventually set to zero). The hard cross-section $\hat{\sigma}^{(\mathrm{n})}_{\mathrm{ab\to X}}$ is then obtained by iteratively(recursively) inverting the Equation A.1 (c.f. [9]).

Let us illustrate how this approach was applied in this paper by explicitly considering the $gg \to Z^0/\gamma^* b\bar{b}$ process. At order α_s^2 (n=2) we get from equation A.1:

$$\begin{aligned}
\sigma^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}} &= f^{(0)}_{g/g} \otimes \hat{\sigma}^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}} \otimes f^{(0)}_{g/g} \\
&+ \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \hat{\sigma}^{(1)}_{\mathrm{Hg\to Z^0/\gamma^*\,H}} \otimes f^{(0)}_{g/g} \\
&+ \sum_{H=b,\bar{b}} f^{(0)}_{g/g} \otimes \hat{\sigma}^{(1)}_{\mathrm{g\bar{H}\to Z^0/\gamma^*\,\bar{H}}} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}) \\
&+ \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \hat{\sigma}^{(0)}_{\mathrm{H\bar{H}\to Z^0/\gamma^*}} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}),
\end{aligned} \tag{A.5}$$

[2] In the paper [9] also final state evolution (i.e. fragmentation functions) are considered but in this paper we limit ourselves to the initial state evolution only, as stated several times in the paper. Subsequently, our choice of processes considered is constrained by this limitation.

which exhausts the possible combinations. The order n=1,2 hard cross sections $\hat{\sigma}^{(0,1)}$ still need to be determined so we move our the procedure first one order down to n=1 and obtain ($H = b, \bar{b}$):

$$
\begin{aligned}
\sigma^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} &= f^{(0)}_{H/g} \otimes \hat{\sigma}^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} \otimes f^{(0)}_{g/g} \\
&+ f^{(0)}_{H/g} \otimes \hat{\sigma}^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}), \\
\sigma^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} &= f^{(0)}_{g/g} \otimes \hat{\sigma}^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} \otimes f^{(0)}_{\bar{H}/g} \\
&+ f^{(1)}_{H/g}(\mu_{1H}) \otimes \hat{\sigma}^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(0)}_{\bar{H}/g},
\end{aligned}
\tag{A.6}
$$

which still cannot be inverted so we move subsequently to n=0 and obtain:

$$
\sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} = f^{(0)}_{H/g} \otimes \hat{\sigma}^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(0)}_{\bar{H}/g} = \hat{\sigma}^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*}\,,
\tag{A.7}
$$

in which case the hard and perturbative cross sections are equal, meaning:

$$
\hat{\sigma}^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} = \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*}\,.
\tag{A.8}
$$

Inserting this result back into Equation A.6 one can now express the hard cross-section:

$$
\begin{aligned}
\hat{\sigma}^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} &= \sigma^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} \\
&- \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}), \\
\hat{\sigma}^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} &= \sigma^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} \\
&- f^{(1)}_{H/g}(\mu_{1H}) \otimes \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*}\,,
\end{aligned}
\tag{A.9}
$$

and now these results finally into Eq. A.5, giving:

$$
\begin{aligned}
\hat{\sigma}^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}} &= \sigma^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}} \\
&- \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \left[\sigma^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} - \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}})\right] \\
&- \sum_{H=b,\bar{b}} \left[\sigma^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} - f^{(1)}_{H/g}(\mu_{1H}) \otimes \sigma^{(0)}_{\mathrm{\bar{H}H}\to \mathrm{Z}^0/\gamma^*}\,,\right] \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}) \\
&- \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}),
\end{aligned}
\tag{A.10}
$$

$$
\begin{aligned}
&= \sigma^{(2)}_{gg\to Z^0/\gamma^* b\bar{b}} \\
&- \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \sigma^{(1)}_{\mathrm{Hg}\to \mathrm{Z}^0/\gamma^*\,\mathrm{H}} \\
&- \sum_{H=b,\bar{b}} \sigma^{(1)}_{\mathrm{g\bar{H}}\to \mathrm{Z}^0/\gamma^*\,\mathrm{\bar{H}}} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}) \\
&+ \sum_{H=b,\bar{b}} f^{(1)}_{H/g}(\mu_{1H}) \otimes \sigma^{(0)}_{\mathrm{H\bar{H}}\to \mathrm{Z}^0/\gamma^*} \otimes f^{(1)}_{\bar{H}/g}(\mu_{2\bar{H}}).
\end{aligned}
\tag{A.11}
$$

As one can observe from Equations A.8,A.9 and A.11 the hard cross section can be expressed as the difference of the perturbative cross section and a subtraction term:

$$\hat{\sigma}^{(n)} = \sigma^{(n)} - \sigma^{(n)}_{\rm subt}. \tag{A.12}$$

Let us stress again that in this approach the M_H is left at non-zero value in all the above terms, contrary to the conventional approach where M_H is eventually set to zero.

It should be emphasized that in this paper only Born-level (tree-level) pQCD calculations were used, thus implicitly assuming that there are no divergences beyond massive ones present for the process at hand. As a consequence, all contributions involving the additional participation of (soft) gluons in the final state X, which would require explicit NLO (loop) calculations, are not considered.

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